Collecting and Characterizing Validation Data to Support Advanced Simulation of Nuclear Reactor Hydraulics

Nam Dinh

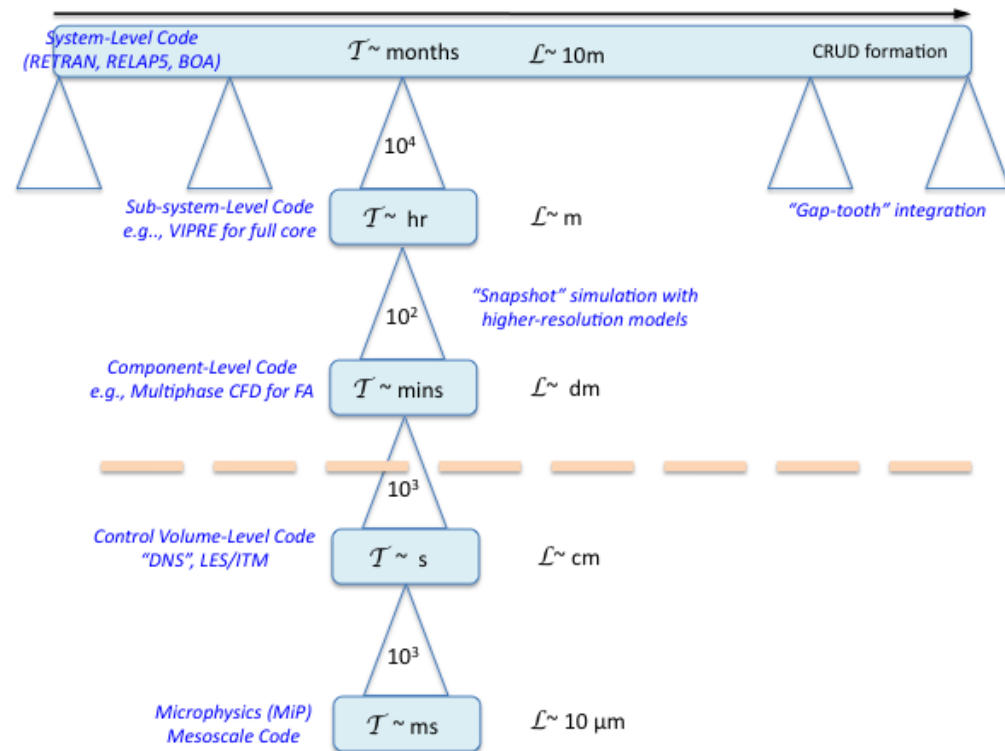North Carolina State University
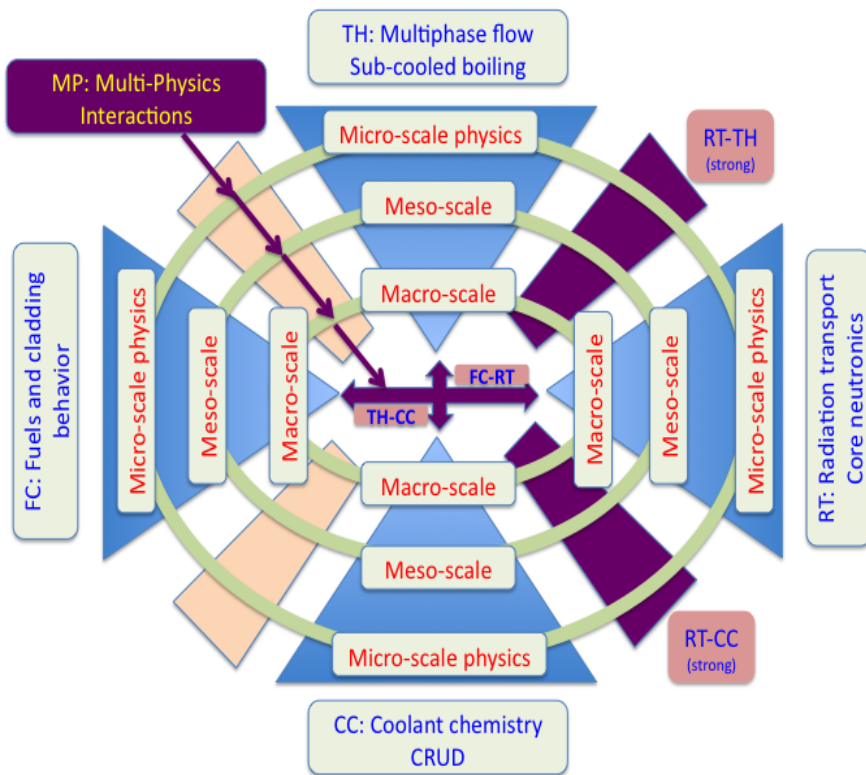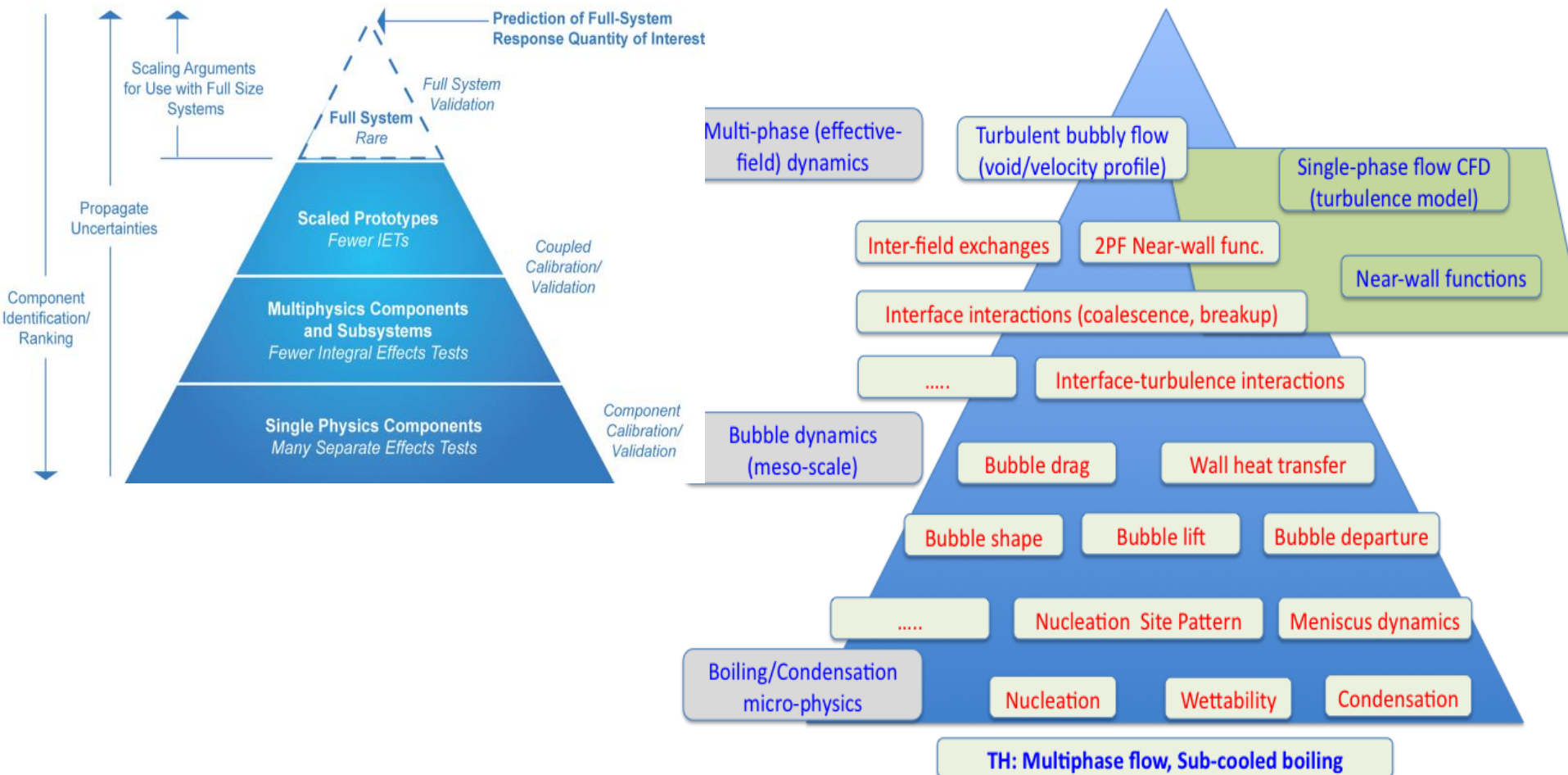
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Idaho National Laboratory

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ASME 2013 Verification and Validation Symposium

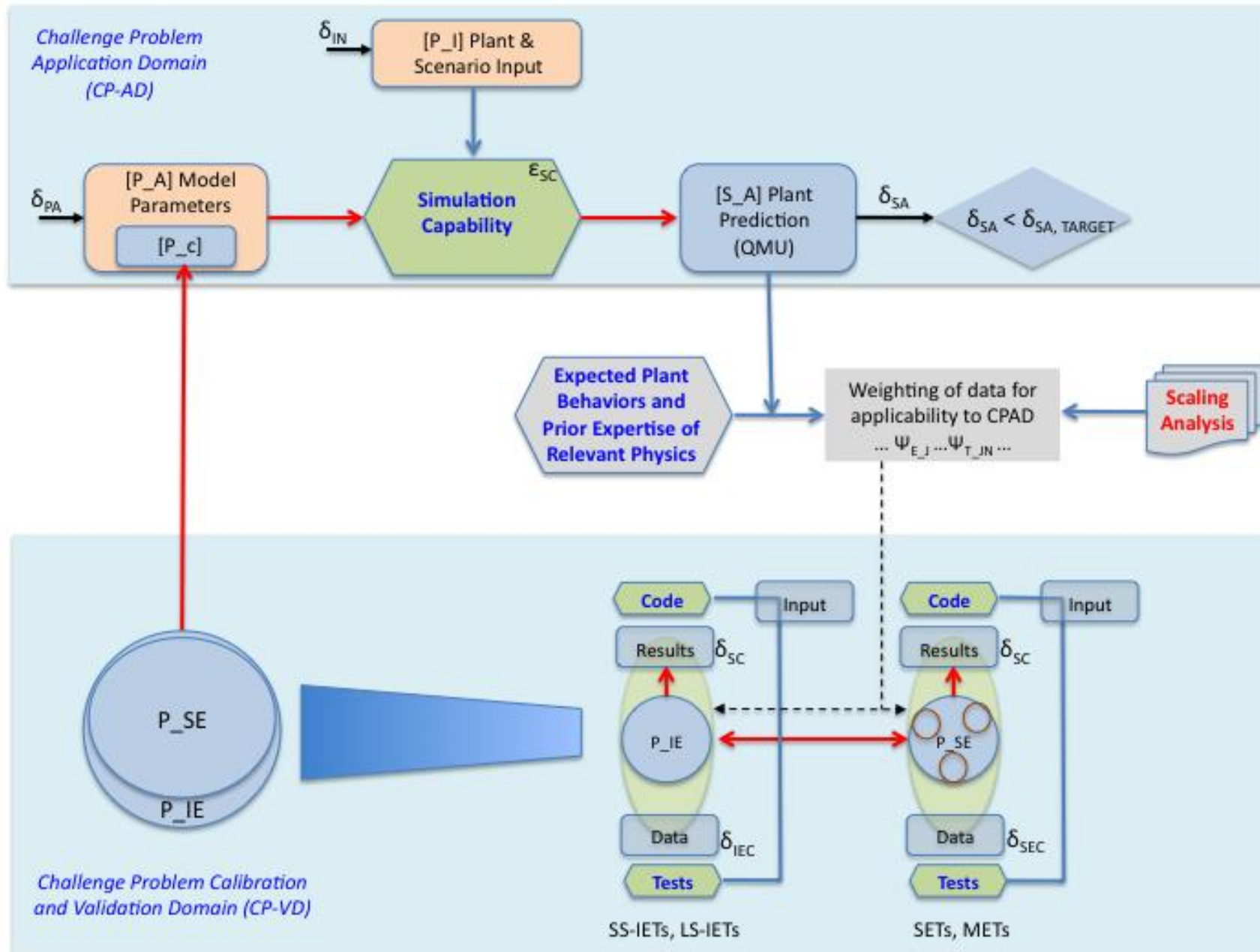Las Vegas, NV, May 22-24, 2013
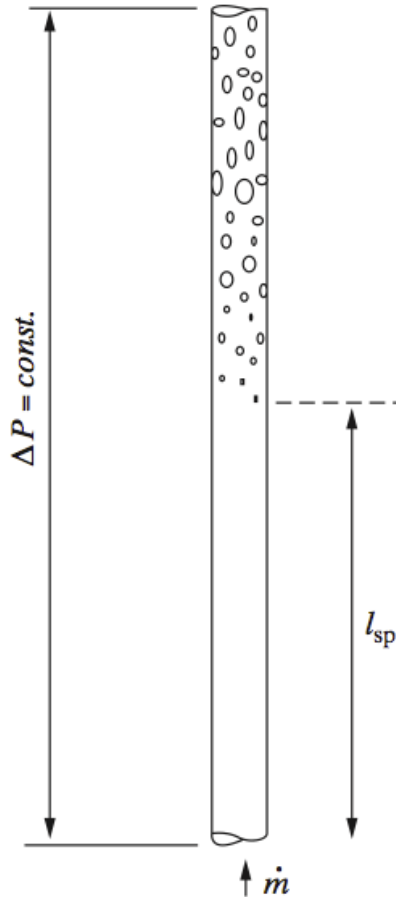
Multi-Physics, Multi-Scale Problem

Validation Hierarchy (Validation Pyramid) of Subcooled Boiling Flow Model

# Bayesian Framework for Data Integration

Nuclear System Analysis – Subcooled Boiling Flow Example

$\Delta P = const.$

l_{sp}

$\dot{m}$

- Underlying physics and models
  - Two-phase flow dynamics – drift-flux/two-fluid model
  - Subcooled boiling
    - Wall heat transfer – mixed forced convection and boiling heat transfers
    - Evaporation at wall – onset of nucleation, onset of significant void, nucleation density, bubble detachment radius and rate
  - Condensation in subcooled bulk fluid
- Data
  - Mostly at macro level, *i.e.*, void fraction distribution, input/output pressure/temperature/flow rate
 - Mostly obtained at conditions (pressure, flow rate heat flux) much different from plant conditions

# Sub-cooled Flow Boiling – Complex Modeling
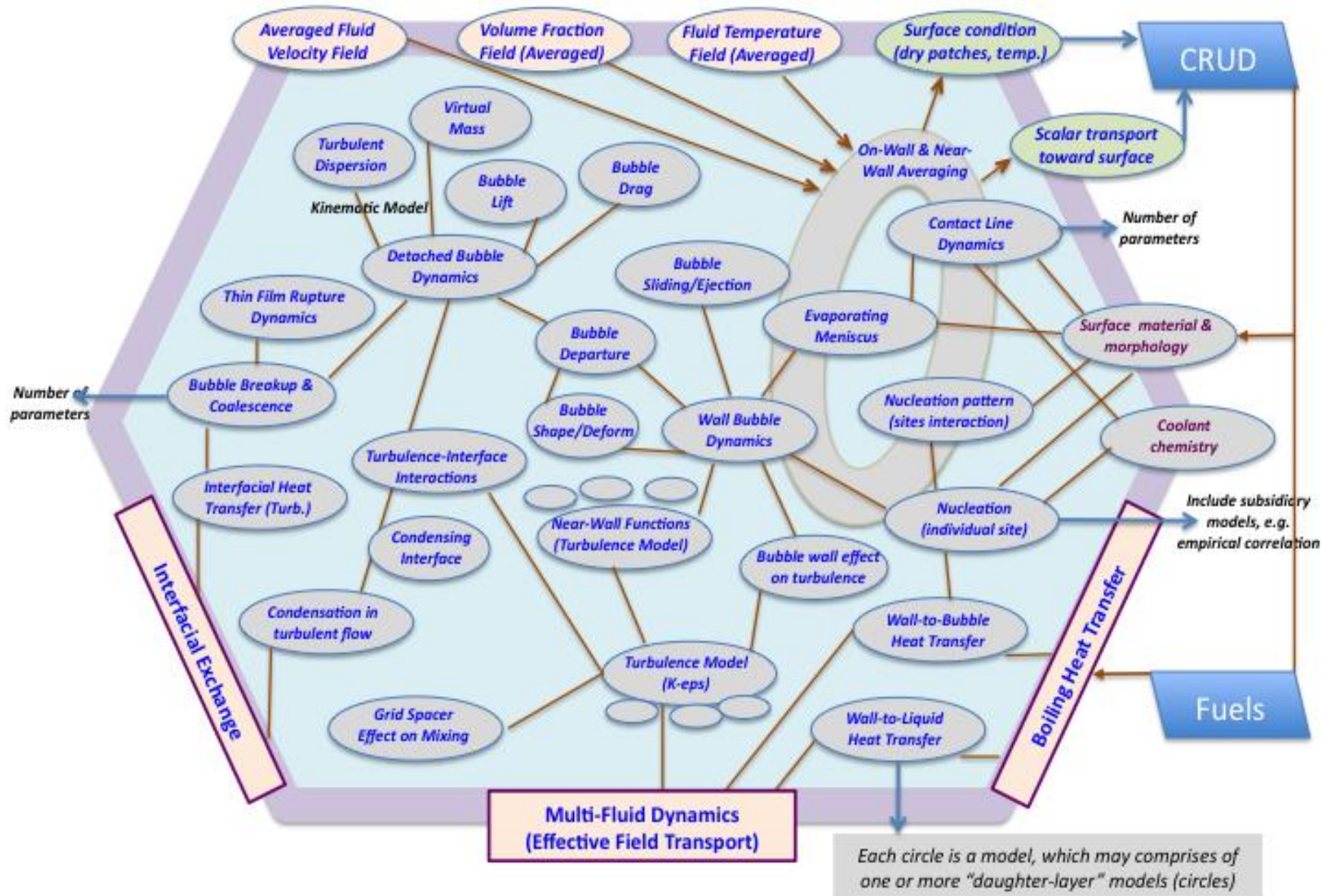
Data Sources

Low pressure

Authors	Geometry (m) D or Dh	Pressure (kPa)	Heat flux (MW m^{-2})	Mass flux (kg m^{-2} s^{-1})	Measurement instrument
Ferell (1964)[a]	Circular 0.0118	410	0.36	540–1060	–
Costa (1967)[a]	Rectangular 0.0038–0.0066 Circular 0.006	174–499	1.0–4.2	3000–7500	–
Staub (1968)[a]	Rectangular 0.01??	110–300	0.31–0.79	320–2800	Gamma-ray
Whittle and Forgan (1967)	Rectangular 0.00? Circular 0.0064				
Evangelisti and Lupoli (1969)	Annular 0.006				
Sekoguchi et al. (1974)	Circular 0.0136–0				
Edelman and Elias (1981)	Circular 0.0113				
McLeod (1986)	Annular 0.0089–0				
Rogers et al. (1987)	Annular 0.0089				
Dougherty et al. (1990a,b)	Circular 0.0091–0				
Bibeau and Salcudean (1994a,b)	Annular 0.0091				
Zeitoun and Shoukri (1997)	Annular 0.0127				
Bartel et al. (1999)	Annular 0.0195				

High pressure

Author	Geometry (m) D or Dh	Pressure (kPa)	Heat flux (MW m^{-2})	Mass flux (kg m^{-2} s^{-1})	Measurement instrument
Bartolemei and Chanturiya (1967)[a]	Circular 0.0154–0.0240	1500–4500	0.38–0.80	870–900	Gamma-ray
Bartolemei et al. (1982)	Circular 0.012	3000–14 800	0.34–2.20	440–2200	Gamma-ray
Christensen (1961)[a]	Rectangular 0.0178	2760–6890	0.21–0.50	640–850	–
Dix (1971)	Annular 0.00914	314–848	0.004–0.03	65–140	Hot-film anemometer, photography
Egen et al. (1957)[a]	Rectangular 0.00475	13 800	0.25–1.60	400–870	
Griffith et al. (1958)	Rectangular 0.0127	8270–13 800	0.31–1.90	450–870	Photography
Labuntsov et al. (1984)	Circular 0.012	2000–7000	0.58–1.2	850–3000	Gamma-ray
Martin (1972)	Rectangular 0.0038–0.0053	7848	0.4–1.7	750–2200	X-ray
Rouhani (1965)[a]	Annular 0.013	980–5000	0.3–1.20	130–1200	–
Mauer (1960)	Rectangular 0.0041	8550–14 300	0.79–7.70	560–4800	Diff pressure, gamma-ray
Celata et al. (1997)	Circular 0.008	1000–2500	0–14	4400–8400	Differential pressure
St. Pierre and Bankoff (1967)	Rectangular 0.0178	1400–5500	0.072–0.29	670–880	Gamma-ray

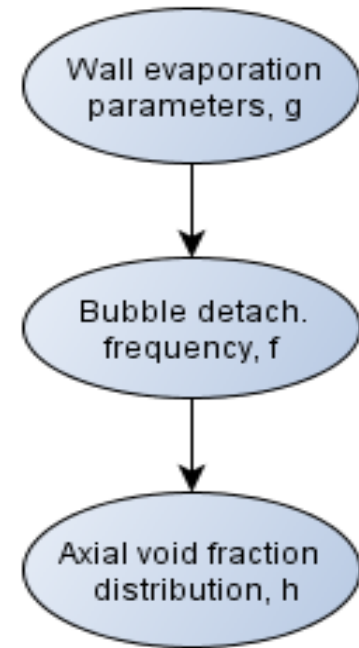# Subcooled Boiling Flows – Data Sources

PTV
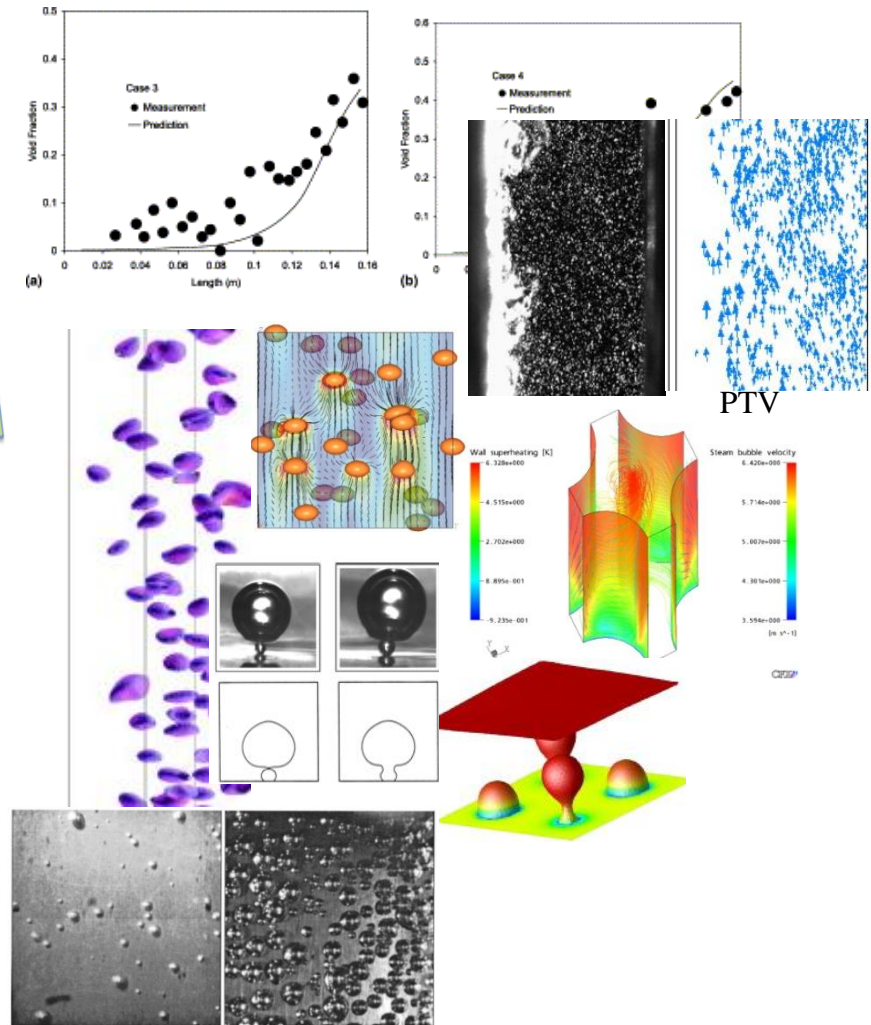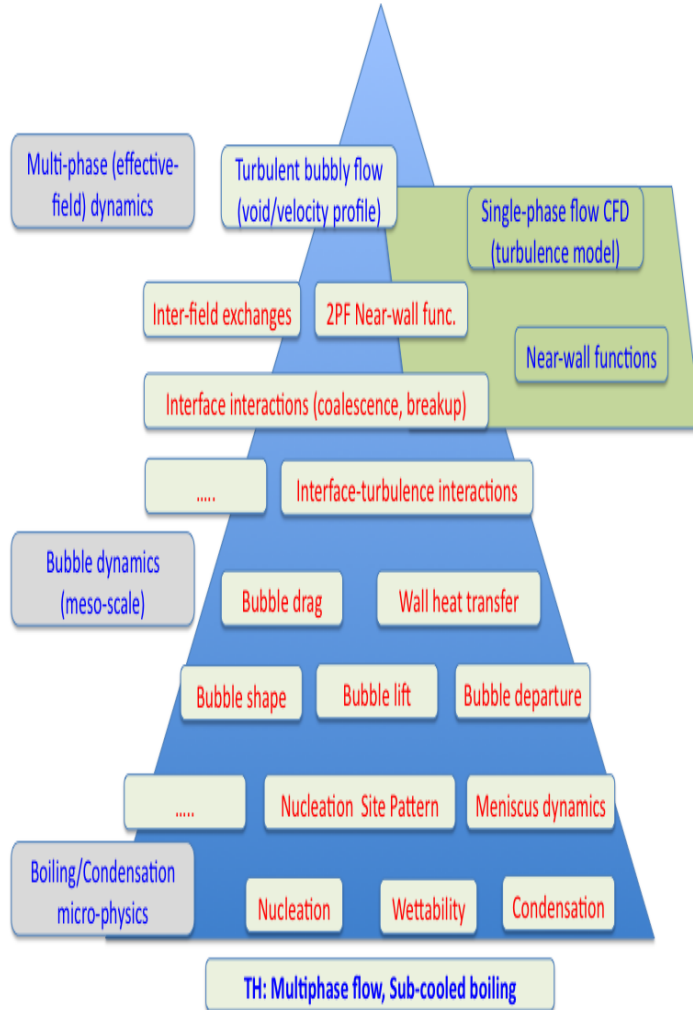
- **Data heterogeneity**: (i) measurement data available at the "system" level – left-most panel – and also at the "sub-model" level – nucleation site density, bubble detachment rate/radius, *etc*. Missing data at some levels; (ii) differences in data scalability, relevancy and uncertainty.

Subcooled Boiling Model Hierarchy
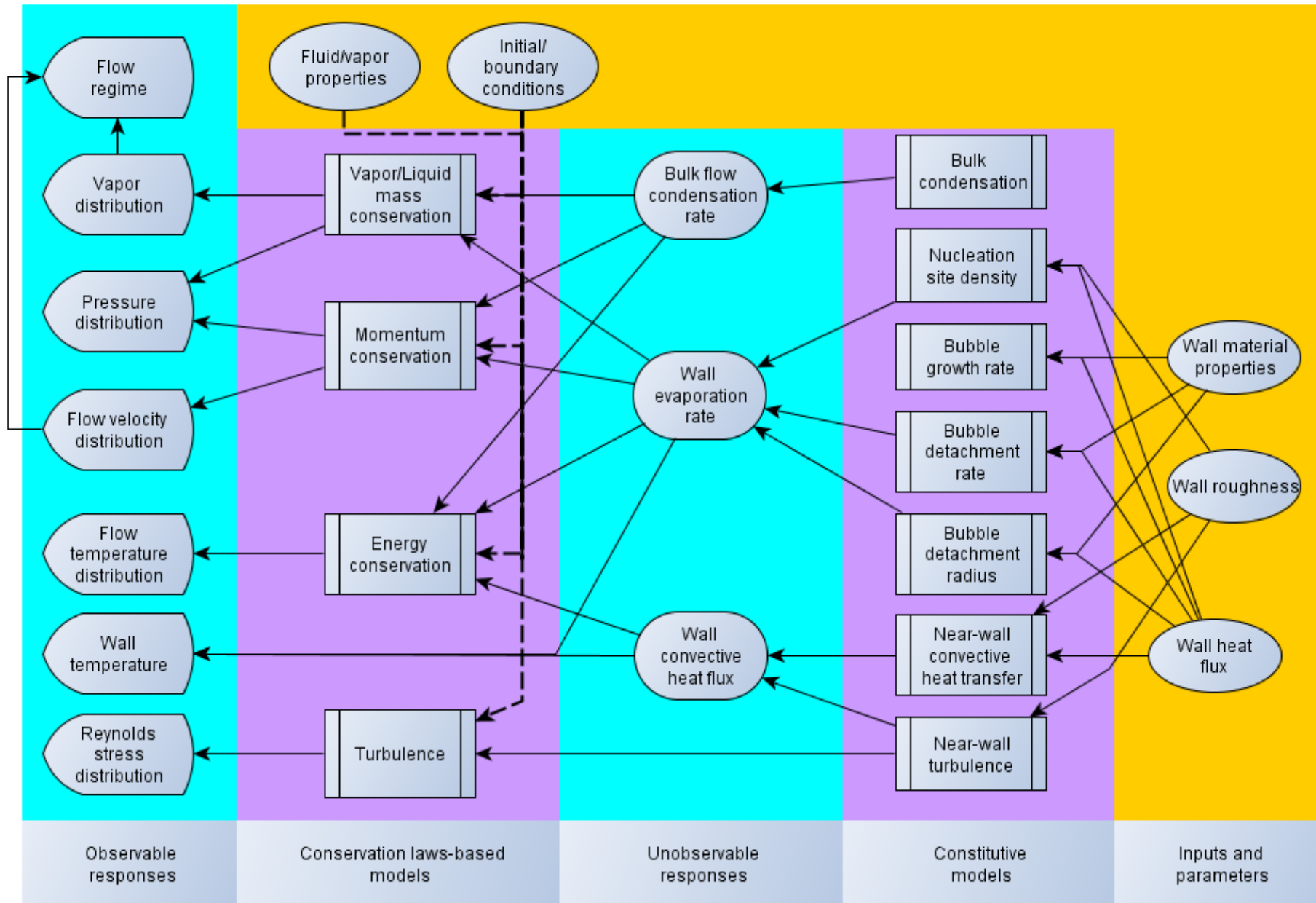
Representation of Multi-physics/Multi-level Subcooled Boiling Flow Model

- Hierarchical regression

- Bayesian influence networks - relationships represented by directed acyclic graphs (DAGs)

- Bayesian Structural Equation Modeling (BSEM) – permits hierarchical/non-hierarchical, recursive/non-recursive structural equations

Subcooled Boiling Flows – Data Heterogeneity
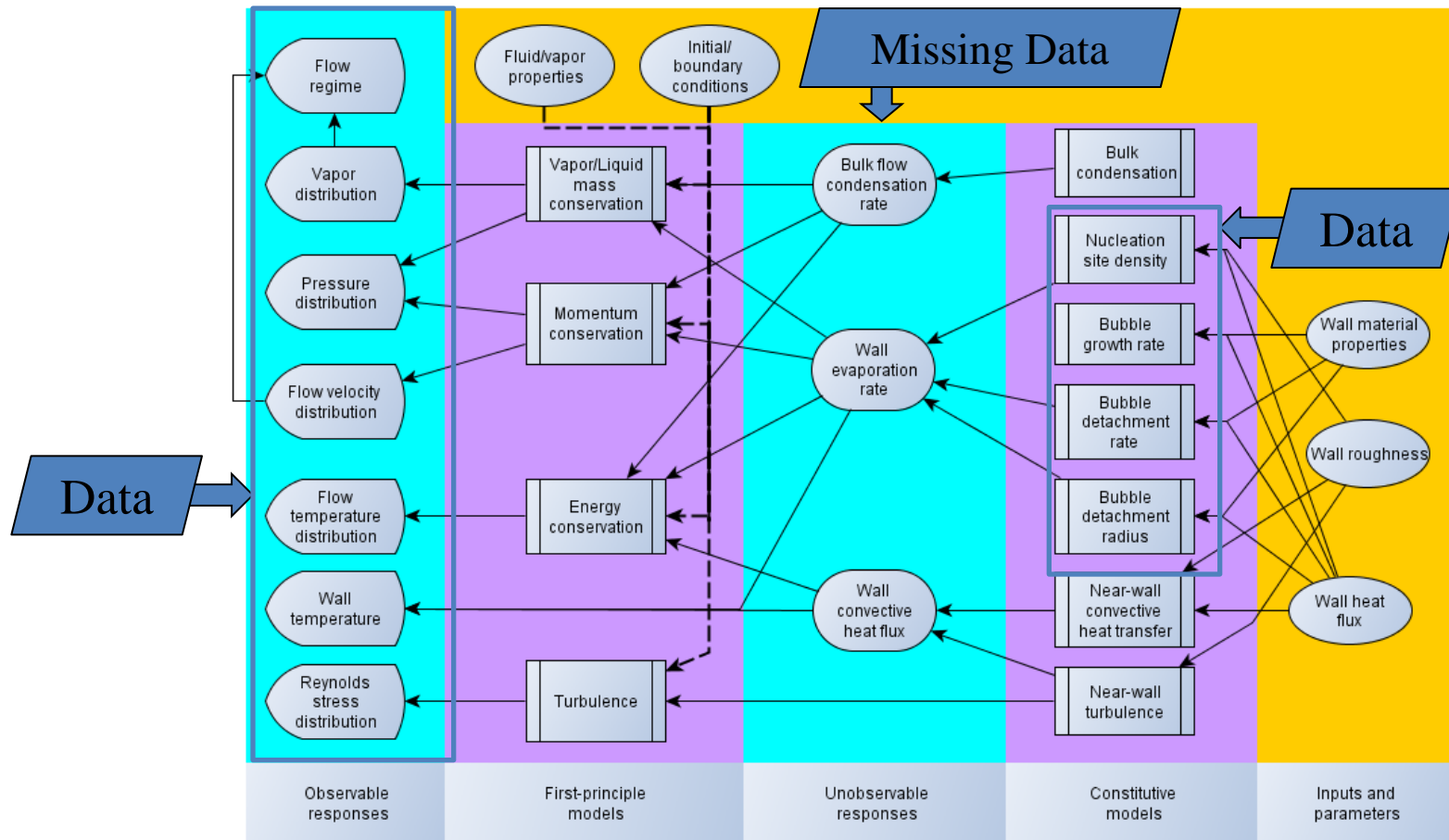
- **Data Identification**
- **Data Collection**
- **Data Review**
- **Data Characterization**
- **Data Assimilation**

Modeling of Multi-Scale & Multi-Physics Subcooled Boiling Flows – Calibration/Validation
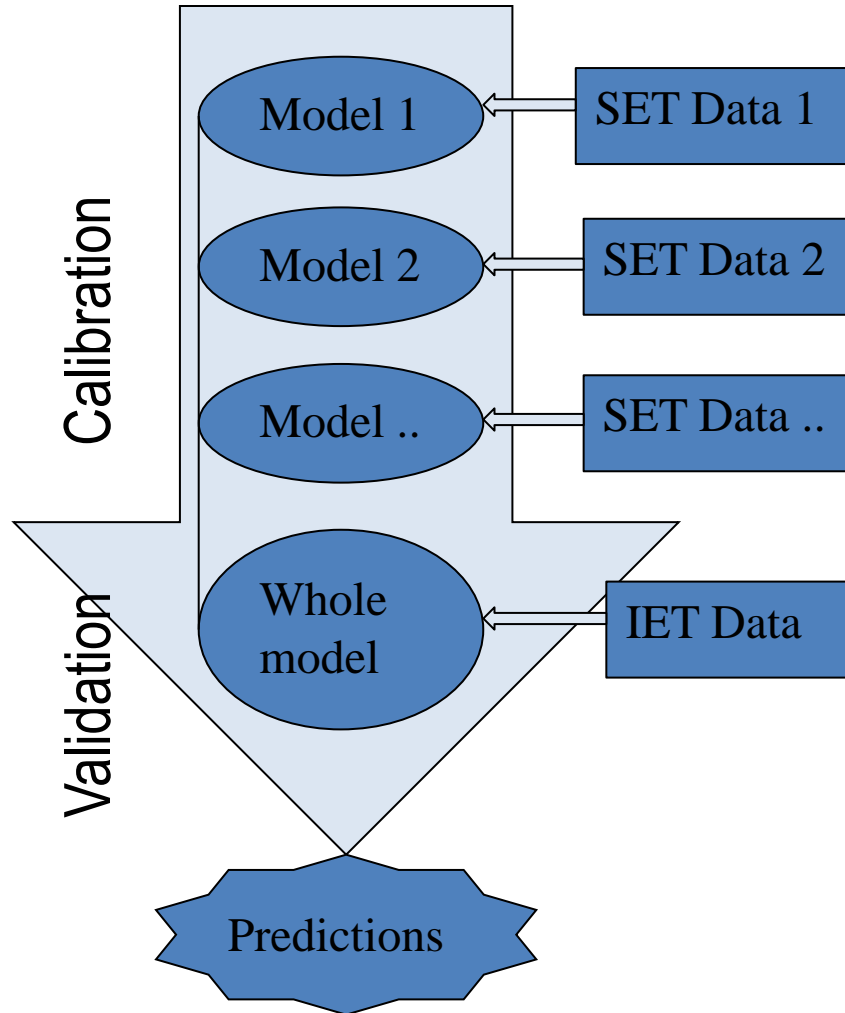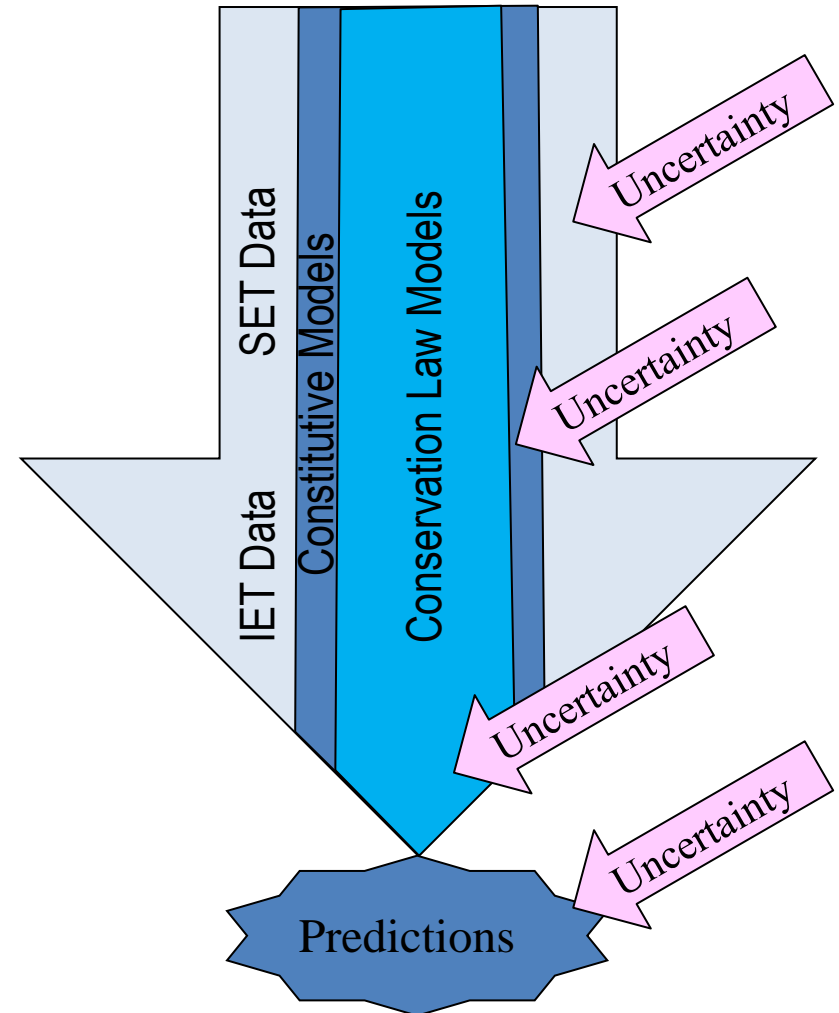
Flow of information in traditional approach to calibration of multi-physics models

"Total data model integration" approach

The Total Data-Model Integration Approach for Model Calibration, Validation and Uncertainty Quantification

- Technical implementation of the proposed "total model-data integration" approach is difficult as it requires a combining of multiple heterogeneous data streams and dealing with multidimensional, multivariate model inputs/outputs.

- A preliminary realization of the approach was delineated in this presentation and employs a range of statistical modeling methods and techniques:

  - Surrogate model construction using a process convolution technique based Principal Component Analysis (PCA) and Gaussian processes (GPs), and Bayesian calibration using Markov Chain Monte Carlo (MCMC) sampling.

- Extension of this approach is envisioned to allow the use of 2D/3D data and data of other scale levels (from SETs) in calibration, validation, and uncertainty quantification of models of higher dimensionality. While proposed and developed for the subcooled flow boiling case study, this approach is intended to be applicable without much modification in the development of any multi-physics models and software.

- The proposed calibration, validation, and uncertainty quantification approach, while offering some flexibility in data usage (*i.e.*, allowing the use of data of different origins, types, quality, *etc.*), does impose requirements on data collection, validation and characterization.

Strategy for Quantification of Data Needs, Data Collection, Validation, and Characterization

- With the total data-model integration approach for model calibration, validation and uncertainty quantification as proposed, data are desirable to be accompanied with:
  - Information about measurement error estimate and data acquisition/derivation methods – to quantify uncertainty;
  - Information needed for "application-oriented" data valuation – to determine relevancy and scalability.

- Quantification of data value/quality can be based on the following criteria:
  - Relevancy
  - Scalability
  - Uncertainty

- Data classification and characterization can be based on factors, such as:
  - Scope of involved physics and strength of their couplings – turbulence, boiling, heat transfer mode, convection mode, *etc*.; single physics (SETs) or multi-physics (IETs);
  - Temporal/spatial dimensionality and resolution of data;
  - Relevancy (in physics involvement sense) to an application or a scenario of interest – SFB, LOCA, Feed-and-Bleed, *etc*.;
  - Data quality – measurement method, error/uncertainty assessment;
  - Scalability – size, geometry, material properties, pressure, temperature, flow rate, *etc*.

Example of Quantification of Data Needs, Data Classification and Characterization to Support SFB model Validation and Calibration

Notes:

ONB – Onset of Nucleate Boiling
OSV – Onset of Significant Void
CHF – Critical Heat Flux

Indirect – indirect determination
Direct – direct measurement or observation

| Physics			Exp. data acquisition method	Data availability	
				Exp.	DNS
Two-phase fluid dynamics	Turbulence		Direct	●	●
	(Dispersed) phase transport		Direct	●	●
	Wall friction		Indirect	●	
	Two-phase flow instability		Direct	●	
	Mechanical interactions between phases	Drag, Lift, Virtual mass forces	Indirect	●	●
		Interfacial tension force - bubble breakup & coalescence	Direct	●	●
Two-phase heat-mass transfer	Convective heat transfer		Indirect	●	
	Wall heat flux partitioning		Indirect	●	
	Wall evaporation	ONB, OSV	Direct	●	
		Nucleation		●	
		Bubble growth dynamics		●	●
		Bubble detachment		●	●
		Boiling crisis (CHF)	Indirect	●	
	Thermal interactions between phases	Vapor condensation in bulk flow	Indirect	●	

Implication to the CASL Validation and Data Plan Strategy

- A first step forward to implement the CASL "application-oriented, total data assimilation" strategy for multi-physics model calibration and validation

- The proposed Bayesian model calibration and data assimilation framework is intended to realize several goals stated in the CASL validation data plan, in particular,
  - "consistent integrated treatment of uncertainty across physics and scales";
  - "Data Realism" concept, *i.e.*, maximal usage of data of different origins, types, scales and qualities;
  - (continuing) incremental update of models with more data becoming available.

- The framework helps to establish the requirements and templates for data in support of the realization of the "VUQ-guided data collection, characterization & qualification":
  - Model of data inaccuracy/uncertainty should be provided together with data, *i.e.*, distributions instead of ± error range;
  - Conversion/homogenization of data to the formats acceptable to VUQ;
  - Reconciliation of conflicting/contradicting data;
  - Data validation/grading/comparison to provide the "weight" factor of a dataset (to be used in VUQ.

CASL Data Center (CDC)

- The CDC functions include
  - (i) Validation data inventory and warehouse;
  - (ii) VUQ-guided data qualification, and
  - (iii) Data processing for interface with users' data operation, with CASL codes and with VUQ workflow, including data assimilation.
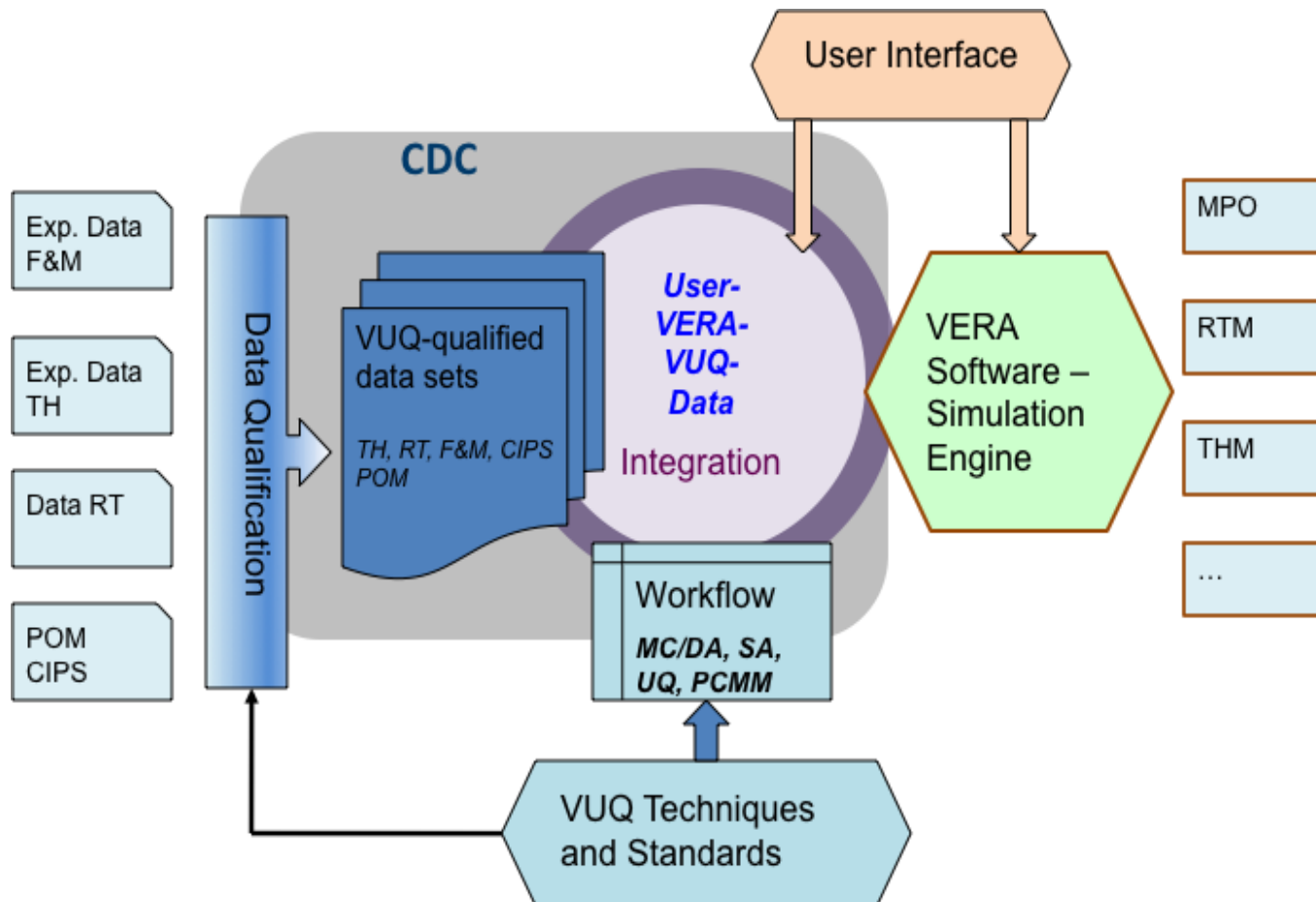
Summary

- "Calibration in the narrow sense may corrupt a model by ignoring information" → a need for "calibration *in the broad sense of combining all relevant information about the parameters" (Jansen & Hagenaars)* (including physically meaningful interpretation of the parameters)

- Validation/calibration of complex multi-physics models using heterogeneous data require a hierarchical representation of interdependency between multiple submodels and parameters.

- Modern nuclear multi-scale multi-physics models are based both on

  – more reliable and scalable conservation laws represented by PDEs

  – less reliable/universal constitutive (closure) laws having a number of tuning parameters

  Both inadequacy of the model form represented by PDEs and uncertainty of model parameters are needed to be assessed in the VUQ process. Closure model parameter calibration needs to be somehow "constrained" by the validity/bias of the conservation laws-based models.

- Data of multi-physics systems are heterogeneous, multivariate, multidimensional and data availability varies greatly depending on scales and physics.

- A total data assimilation approach to VUQ is needed to take the advantage of all available data regardless of their origin, uncertainty and characteristics.

- "Total data-model integration" can be realized with use of model analysis approaches based on Bayesian inference.